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Electron - Phonon Interaction in a Correlated System : A Slave Boson Approach

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Abstract

An analysis of the interplay between electron correlation and electron - phonon (EP) interaction is studied for a low dimensional system. The correlation problem is treated using the Slave - Boson method. The effect of correlation on the EP interaction and the phenomenon of charge density wave (CDW) formation is predominantly determined by the band renormalization factor q. It is shown that in general the electron correlation tends to suppress the CDW state. This has been established by calculating the variation with electronic correlation of the Peierl's instability, the phase diagram, the CDW order parameter and the spectral density function of the collective modes.

Keywords : Slave - Boson, Charge - Density Wave (CDW), Metal - Insulator Tra sition.

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1 Introduction.

The fundamental interactions which are important to determine the electronic properties of strongly correlated fermionic systems are the electron-electron and electron-phonon interactions. But the speculations concerning the interplay between electron-electron and electron-phonon (EP) interactions near the Metal to Insulator transition in doped materials is still controversial. There are several attempts [1] - [5] for such an analysis showing conflicting results ; Zielinski et al [1] following a strong coupling theory arrived at the conclusion that there is an enhancement of T_c (EP coupling constant) around quarter filling of the band due to the presence of strong correlation. On the other hand Kim et al [2] argue that the EP interaction strength decreases with Coulomb correlation, due to the suppression of charge fluctuation as one approaches the metal insulator transition; there are also several other groups ([3] - [5]). Therefore, a proper understanding of the phenomena is still lacking.

For a low dimensional paramagnetic metal it is expected that at half-filling the strong correlation will tend to drive the system towards the Mott-Hubbard insulator, the EP interaction will tend to stabilize the Peierl's transition. Our effort goes to investigate the nature of the interplay of the two interactions. In an attempt to doing so we have used the Slave - Boson formalism within the saddle point approximation which is an effective method to treat the correlation problem. In sec. 2. we have derived an effective EP interaction and hence Peierl's transition in a correlated system as well as the effect of electron correlation on the CDW order parameter are also studied. In conclusion we summarize the main results and discuss the limits of validity of the present report.

2 Electron - phonon interaction in a strongly correlated system:

The minimal model to describe the correlated system is the Hubbard model, but no exact solution is known for the model except in one dimension. The main obstacles encountered to obtain a solution of the Hubbard model is to keep track of the occupancy of a site. The formalism of the Slave - Boson approach to the strongly correlated system introduced by Kotliar and Ruckenstein [6] successfully keeps track of all possible occupancy of a lattice site by means of four auxilliary Boson fields corresponding to a site being empty (e_i), doubly occupied (d_i) or singly ocupied ($s_{i\sigma/-\sigma}$) with a up (σ) or down ($-\sigma$) spin electron, these Boson fields are constrained by the requirements that (i) the total probability of occupation of a site being unity must be conserved and (ii) the total charge at a site is also conserved. In this approximation the Hamiltonian of the system takes the simple form of an effective tight binding model with a modified hopping integral of the form $t_{ij} \rightarrow \tilde{q}t_{ij}$, where the correlation effects are built - in through the multiplicative factor $\tilde{q} = z^{\dagger}z$, z is a function of the Boson operators and it can be expressed as a funtion of effective Coulomb corclation u and the dopant concentration δ in the saddle point approximation [6].

In the presence of small displacement ($\vec{u}_i$) of the atom at site i, t_{ij} can be expanded in a Taylor series and the leading term in the displacement gives rise to the electron-phonon EP interaction Hamiltonian given by,

$$H_{e-p} = g\tilde{q}\sum_{\vec{k}\vec{q}\sigma} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c_{\vec{k}\sigma} A_{\vec{q}} \tag{1}$$

where $A_{\vec{q}} = (b_{\vec{q}} + b^{\dagger}_{-\vec{q}})$ is the q-th Fourier component of the atomic displacement $\vec{u}_i$; with $b_{\vec{q}}(b^{\dagger}_{\vec{q}})$ denoting the phonon annihilation(creation) operator ; and g is the coupling constant. It is evident from equation (1) that within this approximation scheme the entire effect of electron correlation is to modify the EP coupling constant by the multiplicative factor $\tilde{q}$ which amounts to a large reduction in the effective EP coupling constant due to strong correlation [7].

It is well known that the Peierl's instability of a low dimensional metal is brought about by the softening of the phonon (with the wave vector corresponding to the nesting of the Fermi surface) which results in a lattice distortion accompanying the CDW. In order to see how the Peierl's transition is effected by the electron correlation, we calculated [7] the renormalized phonon frequency ($\Omega_{\vec{Q}}$) with wave vector $\vec{Q}$, which corresponds to the nesting of the Fermi surface i.e., $\epsilon_{\vec{k}+\vec{Q}} = -\epsilon_{k}$. The temperature at which the transition ($\Omega_{\vec{Q}} = 0$) takes place is given by

$$\tilde{T}_p = \tilde{q}\exp[-1/\lambda\tilde{q}] \tag{2}$$

where $\lambda = (4g^2N(0)/\omega_{\vec{Q}})$ is the dimensionless coupling constant, $N(0)$ being the density of states at the Fermi energy, $\omega_{\vec{Q}}$ is the phonon frequency in the absence of the EP interaction. Equation (2) essentially gives the phase-diagram in the ($u \sim \tilde{T}$) plane as shown in figure (1) and the system under consideration being at a temperature $T < T_p$ is in the CDW state. It is clear from figure (1) that at low dopant concentration the CDW phase appears for $u < 1$ where, $u = U/U_c$ (U_c being the critical value of U where the system undergo the Metal-Insulator transition) i.e., only in the metallic

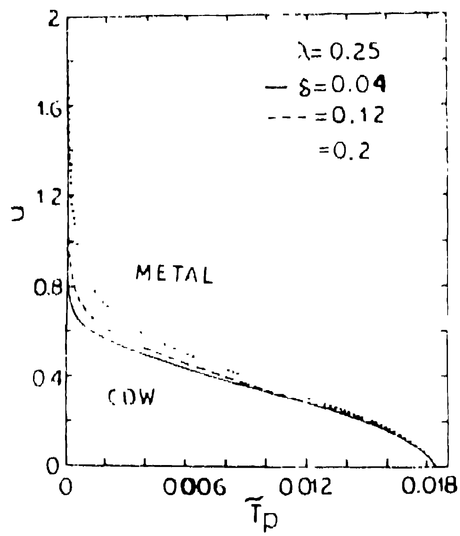

Fig.1. The phase diagram for $\lambda = 0.25$.

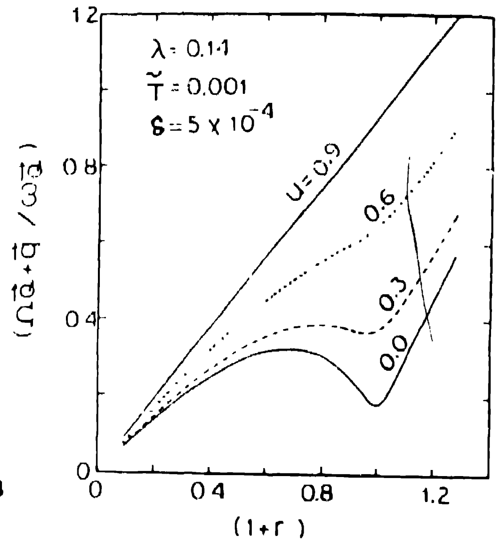

Fig.2. The dispersion of the giant Kohn anomaly phonon in the metallic regime for different u.

regime. But with increasing δ the CDW state persists even at much higher values of u, indicating that there can be a Peierl's instability even in the doped regime ($u > 1$) although the corresponding transition temperatures are much lower.

The behaviour of the giant Kohn anomaly as a function of the correlation or the dopant concentration is studied in [7]. The figure 2. shows the u and δ dependence of $\Omega_{\vec{Q}+\vec{q}}/\omega_{\vec{Q}}$ with $(1+r)$, where $r = q/Q$ and $|\vec{q}| \ll |\vec{Q}|$. The figure 2. shows that in the absence of correlation there is a softening of the Qth phonon at a particular temperature for a given EP coupling constant. On increasing the value of u, the Kohn anomaly is suppressed, which indicates that correlation effect suppresses the Peierl's instability in the metallic regime whereas in the doped regime it can be shown [7] that in the Mott-Hubbard insulating state the system cannot undergo Peierl's transition, as it is metallised by increasing δ, it becomes prone to the Peierl's instability.

The CDW state is characterised by the non - vanishing expectation value of the phonon amplitude corresponding to the particular value of the wave vector $\vec{q} = \vec{Q}$

i.e., $< A_{\vec{Q}} > \neq 0$. In the CDW state the quasiparticle energy spectrum develops a gap Δ at the Fermi energy. From the saddle - point Hamiltonian and within the weak coupling limit it is given by

$$\Delta \equiv g < A_{\vec{Q}} > = 2\omega_c \exp[-1/\lambda\bar{q}] \tag{3}$$

where λ is the dimensionless coupling constant in the CDW state, ω_c is the cut-off frequency which determines the range of energy around the Fermi level beyond which the nesting property is destroyed. The figure 3. shows the variation of CDW - gap parameter with the electronic correlation for different values of δ. The gap decreases rapidly in the begining with increasing value of u, but then it slowly vanishes with increasing u, which shows that as $U \rightarrow U_c$ the localization of the electrons inhibits the formation of the CDW state. In the doped regime with increasing δ, the critical value of u (below which CDW state exists) increases and the CDW order parameter grows on. This is in contradiction with the results obtained by Deeg et al [4] where the CDW order parameter decreases with increasing δ, probable cause for this discrepancy will be discussed later.

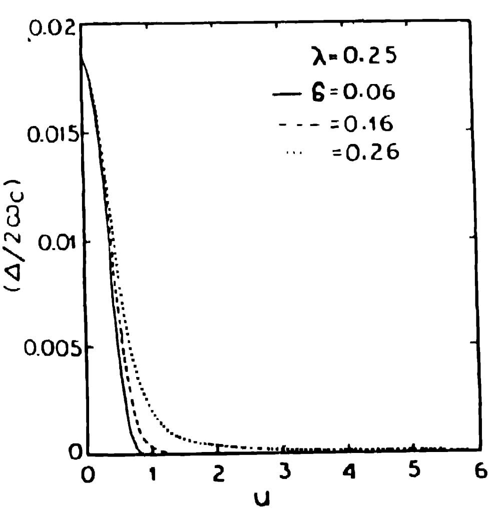

Fig.3. The variation of the CDW gap with u for $\lambda = 0.25$.

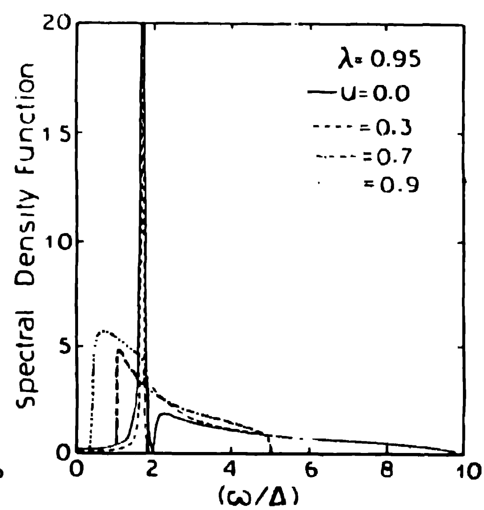

Fig.4. Spectral density function for the CDW amplitude mode for $\lambda = 0.95$ and different u.

It is well known that fluctuation of the phase and the amplitude of the order parameter results in the appearence of the collective modes of the system. The amplitude mode is a measure of the CDW order parameter (Δ), which has a frequency $\omega_{AM} = 2\Delta$ at zero wave vector. Therefore, it is worthwhile to investigate the effect of electron correlation on the CDW-amplitude mode. The frequency of the amplitude mode and its spectral density function can be calculated from the amplitude response function [7]. The frequency of the amplitude mode turns out to be

$$\omega_{AM} = 2\tilde{q}\Delta \tag{4}$$

Since the band renormalization factor $(\tilde{q})$ decreases with increasing value of the intratomic Coulomb repulsion (U), the CDW-amplitude mode frequency will also decreas with increasing u. The spectral density function is expected to show a peaked structure around ω_{AM}. It can be seen from the figure 4. that for vanishing u the spectral density function has a well defined peak corresponding to the CDW-amplitude mode at a frequency slightly less than 2Δ followed by a broad asymmetrical hump. On increasing u this peak shifts to lower frequency while its width decreases, and the hump becomes more prominant with increasing strength. Further increasing u the peak vanishes and the hump further gains in strength. This clearly signifies the suppression of the CDW state as the system is driven towards the Mott-Hubbard insulator due to electronic correlation. On the other hand in the doped regime a similar behaviour of the spectral density function results on lowering the dopant concentration δ. At larger values of δ a well defined peak corresponding to the CDW-amplitude mode exists, which vanishes on going to smaller values of δ. This again is an indication of the fact that the CDW state is suppressed in the low dopant concentrations in the doped regime. This result is physically understandable in the sense that in the doped regime (i.e, $u > 1$) for $\delta = 0$, the system is a Mott insulator, hence there is no possibility for a transition to the CDW-state.

3 Conclusion

In summary, we analysed the effect of electron correlation (u) on various facets of EP interaction such as the coupling constant (λ), the on set of Peierl's instability, the $(u \sim \tilde{T}_p)$ phase diagram, the CDW order parameter and the collective modes of the CDW state. The correlation effect enters the calculation through the band renormalization factor $\tilde{q}$, which also depends on the dopant concentration δ. The dependence of $\tilde{q}$ on u and δ has been discussed in [7]. In the limit of $\delta = 1$, which corresponds to an empty band in the case of hole doping and a full band in the case of electron doping, $\tilde{q}$ takes the value unity idetically [7]. This is an artifact of the saddle point approximation, hence these results make sense only for more than half-filling of the lower Hubbard band, for the case of hole doping.

In the present calculation the possibility of reduction in the nesting of the Fermi surface with increasing δ has not been accounted for. That may be causing the contradiction in the δ-dependence of the CDW order parameter with the results obtained by Deeg et al [4], where the order parameter decreases with increasing δ.

In the CDW state the Brinkman - Rice parameter U_c differs from its value in the paramagnetic state [7] where, U_c depends on the order parameter. We see in the present paper that the CDW order parameter also depends on U_c through $\tilde{q}$ as is evident from equation (3). So it requires a self-consistent calculation.

Lastly, these results are within the mean-field approximation; the inclusion of the effect of fluctuations may alter the results. This is under present investigation and will be reported elsewhere.

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